Available Online

J. Sci. Res. **16** (2), 589-602 (2024)

**JOURNAL OF**

**SCIENTIFIC RESEARCH**

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**Publications**

Volumetric and Ultrasonic Properties of Liquid Mixtures of Ethyl Benzene with Alkanols at Different Temperatures

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Received 4 December 2023, accepted in final revised form 6 March 2024

Abstract

The densities (*ρ*), and ultrasonic speeds (*u*) of pure ethyl benzene, 1-butanol, 1- pentanol, and those of their binary mixtures, with ethyl benzene as a common component, covering the whole composition range have been measured at 298.15, 303.15, 308.15, 313.15, 318.15 and 323.15 K. From the experimental data the excess molar volume (*V*mΕ), deviations in isentropic compressibility (∆*κs*) and deviations in ultrasonic speed (∆*u*) have been determined. The sign and magnitude of these parameters were found to be sensitive towards interactions prevailing in the studied systems. The excess or deviation properties (*V*mΕ, Δ*u*, or ∆*κs*) have been correlated using a Redlich-Kister type equation to obtain their coefficients and standard deviations. The variations of derived parameters mentioned above with composition offer a convenient method to study the nature and extent of interactions between the component molecules of the liquid mixtures, which are not easily obtained by other means.

*Keywords*: Density; Speeds of sound; Ethyl benzene; 1-Butanol; 1-Pentanol; Binary mixtures; Interactions.

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doi: [https://dx.doi.org/10.3329/jsr.v16i2.70220](http://dx.doi.org/10.3329/jsr.v16i2.51841) J. Sci. Res. **16** (2), 589-602 (2024)

1. Introduction

The measurements of thermodynamic properties of binary liquid mixtures of aromatic compound and 1- alkanols as one of the components have been employed in understanding the nature of molecular systems and physiochemical behavior of binary liquid mixtures are useful in process engineering design and other related applications [1-4], and have drawn considerable attention in recent years [5-12]. However, the literature survey on the thermodynamic and acoustic properties of binary mixtures containing aromatic hydrocarbon and 1-butanol or 1-pentanol reveals that the databases are limited. It is, therefore, quite essential in this area of research to carry out systematic investigations involving the physical properties of the binary mixtures containing aromatic hydrocarbon and 1-butanol or 1-pentanol. As a part of our ongoing research [13-20]on the accumulation of the physical property data of organic liquid mixtures focused on the competitive complexation and self-association that may occur in the mixed system of the aromatic hydrocarbon with 1-butanol or 1-pentanol.

1-alkanol was chosen as a solvent for the present study because its properties were the subject of considerable interest due to the versatility of this compound as a solvent for cosmetics, fragrances, and flavoring agents. Ethyl benzene (EB) is also a well-known organic solvent used in many industrial and biological processes. This also aims to understand the intermolecular interactions, particularly the (π….. H) bonding between the molecules of n-alkanols and aromatic hydrocarbons, with their strength influenced by the size, shape, and chemical nature of component molecules. 1-butanol or 1-pentanol is protic and exists in associated forms, whereas EB is aprotic and, thus, exhibits no hydrogen bonding.

In order to investigate the nature of interactions, we have measured the densities (*ρ*), and ultrasonic speeds (*u*) of the binary mixtures of EB with 1-butanol or 1-pentanol, including those of pure liquids at T= (298.15, 303.15, 308.15, 313.15, 318.15, 323.15) K covering the entire composition ranges expressed by the mole fraction x2 of 1-butanol or 1-pentanol. From the experimental values of *ρ* and *u*, excess molar volumes (*V*mE), deviations in isentropic compressibility (Δ*κS*), and ultrasonic speeds (Δ*u*) have been calculated. The Redlich-Kister polynomial [21] was fitted to the excess or deviation properties to derive the binary coefficients and the standard errors between the experimental and the calculated quantities. Saleh *et al.* [22] have determined *V*mE and *η*E values for binary mixtures (1-propanol or 2-propanol or 1-butanol or t-butanol + cumene) at T = (303.15 to 323.15) K while Bhatia *et al.* [23]studied densities, speed of sound and isentropic compressibilities for the binary mixtures of (1-decanol + *o*-xylene, + *m*- xylene, + *p*- xylene, + ethyl benzene, and + mesitylene at T = (298.15, and 308.15) K while, Gahlyan *et. al.* [24] measured *V*mE for binary mixtures (1-propanol+benzene or toluene or *o*- or *m*- or *p*-xylene) at T= 303.15K. However, to the best of our knowledge, no experimental values of densities, viscosities, and ultrasonic speeds or the corresponding derived properties have been reported in the literature for the mixed systems of 1-butanol or 1-pentanol with EB at (298.15, 303.15, 308.15, 313.15, 318.15, 323.15)K. Therefore, the objective of the current work was to create the binary mixed systems of 1-butanol or 1-pentanol and ethyl benzene covering the entire miscibility range and to measure the aforementioned thermophysical properties of the mixtures considering the lack of data regarding the composition-temperature dependent mixing behavior in such systems.

**2. Experimental**

**2.1. *Materials***

1-Butanol, 1-pentanol and Ethyl Benzene are purchased from Sigma-Aldrich with a molar percentage purity higher than 99. Materials were used without further purification. The purity of substances was checked by comparing their density with the literature data given in Table 2. The agreement between the experimental and literature data is acceptable.

Table 1. Specifications of the components in binary mixtures.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Chemical name | Source | CAS no. | Initial purity  (mass fraction) | Purification method |
| Ethyl benzene | Sigma-Aldrich | 100-41-4 | 0.998 | none |
| Butan-1-ol | Sigma-Aldrich | 71-36-3 | 0.998 | none |
| Pentan-1-ol | Sigma-Aldrich | 71-41-0 | ≥0.99 | none |

Table 2. Comparison of experimental densities, *ρ*exp of pure liquids with literature values at *T* = (298.15, 303.15, 308.15, 313.15, 318.15, and 323.15) K.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Liquid (s) | *T*/K | *ρ*exp·10−3/kg·m−3 | |  |
| Exp. | Lit. | Ref. |
| Ethyl benzene | 298.15 | 0.862048 | 0.862433 | [32] |
|  | 303.15 | 0.857594 | 0.85815 | [11] |
|  | 308.15 | 0.851102 | 0.8535 | [33] |
|  | 313.15 | 0.848752 | 0.8495 | [33] |
|  | 318.15 | 0.844322 | 0.8447 | [33] |
|  | 323.15 | 0.839846 | 0.84038 | [11] |
| Butan-1-ol | 298.15 | 0.806954 | 0.80613 | [[3](file:///C:\Users\USER\Downloads\V6_EB+Alkanol_IMR%20Edit%20(1).docx#_ENREF_34)4] |
|  | 303.15 | 0.802900 | 0.80228 | [34] |
|  | 308.15 | 0.79800 | 0.79804 | [35] |
|  | 313.15 | 0.79509 | 0.7946 | [36] |
|  | 318.15 | 0.791126 | 0.79097 | [37] |
|  | 323.15 | 0.787126 | 0.7876 | [[3](file:///C:\Users\USER\Downloads\V6_EB+Alkanol_IMR%20Edit%20(1).docx#_ENREF_43)8] |
| Pentan-1-ol | 298.15 | 0.811567 | 0.81103 | [39] |
|  | 303.15 | 0.807875 | 0.8072 | [39] |
|  | 308.15 | 0.804155 | 0.80416 | [40] |
|  | 313.15 | 0.800403 | 0.8000 | [40] |
|  | 318.15 | 0.796615 | 0.79659 | [41] |
|  | 323.15 | 0.792783 | 0.79275 | [41] |

Standard uncertainties: *ρ*exp = 2.9·10–2 kg⋅m–3, *T =*1·10−2 K

**2.2. *Measurements***

Density and ultrasonic speed data from the literature have been used to ascertain the solvent purity (Table 1). Binary mixtures were prepared by mixing a known mass of each liquid in an air-tight and stopped glass bottle. To avoid evaporation and solvent contamination, the solutions were used immediately after preparation. An electronic balance (Mettler Toledo, B204-S, Switzerland) with an accuracy of ± 0.0001 g was used for weighing. The estimated uncertainty in mole fraction was 0.0002. Densities, ρ, and ultrasonic speeds, u of the pure liquids and their binary mixtures have been measured at temperature intervals of 5 K between (298.15 to 323.15) K by using a vibrating tube densimeter and a sound analyzer (Anton Paar DSA 5000) that thermostated within ± 0.01 K. The average uncertainties in the density and speed of sound measurements were ± 2.9·10–2 kg·m–3 and ± 1.3·10–1 m·s–1, respectively. All the measurements were conducted in triplicate and averaged for calculations.

**3. Results and Discussion**

**3.1. *Volumetric properties***

Binary compositions of the mixtures of Ethyl benzene (EB) with 1-butanol and 1-pentanol, the experimental values of density, *ρ*, and excess molar volumes, *V*mΕ, at *T* = (298.15, 303.15, 308.15, 313.15, 318.15 and 323.15) K are summarized in Table 3.

Table 3. Composition, Experimental Densities, *ρ*exp, Excess Molar Volumes, *V*mΕ*,* Experimental Speeds of Sound, *u*exp, Deviation in Speeds of Sound, Δ*u*, Isentropic Compressibility, *κs*, and Deviation in Isentropic Compressibility, Δ*κs*, for the Binary Systems of Ethylbenzene (1) + 1-Butanol (2) at *T* = (298.15, 303.15, 308.15, 313.15, 318.15 and 323.15) K.

|  | *ρ*exp·10−3 | *V*mΕ·106 | *u*exp | Δ*u* | *κ*s·1012 | Δ*κ*s·1012 |
| --- | --- | --- | --- | --- | --- | --- |
|  | / kg⋅m−3 | /m3⋅mol–1 | /m⋅s–1 | /m⋅s–1 | /m2N-1 | / m2N-1 |
| T/K = 298.15 |  |  |  |  |  |  |
| 0.0000 | 0.862048 | 0.0000 | 1266.09 | 0.0000 | 723.6680 | 0.0000 |
| 0.0476 | 0.860002 | 0.00937 | 1254.11 | -10.8617 | 739.3146 | 8.5488 |
| 0.1000 | 0.857691 | 0.01972 | 1243.25 | -20.4586 | 754.3141 | 16.4611 |
| 0.1517 | 0.855341 | 0.03099 | 1232.41 | -30.018 | 769.7510 | 24.8118 |
| 0.2005 | 0.853050 | 0.04347 | 1221.73 | -39.4567 | 785.3713 | 32.1090 |
| 0.2499 | 0.850695 | 0.05266 | 1213.47 | -46.4266 | 798.3035 | 38.3818 |
| 0.3001 | 0.848256 | 0.05940 | 1205.91 | -52.6438 | 810.6738 | 46.2936 |
| 0.3501 | 0.845788 | 0.06229 | 1201.80 | -55.3707 | 818.6044 | 52.9326 |
| 0.4005 | 0.843234 | 0.06464 | 1200.30 | -55.4412 | 823.1373 | 58.8701 |
| 0.4509 | 0.840632 | 0.06364 | 1200.00 | -54.2703 | 826.0980 | 62.9464 |
| 0.5003 | 0.838017 | 0.06144 | 1200.12 | -52.6666 | 828.5101 | 66.8555 |
| 0.5500 | 0.835333 | 0.05619 | 1201.70 | -49.5502 | 828.988 | 68.6798 |
| 0.6003 | 0.832531 | 0.05136 | 1203.36 | -46.2887 | 829.4848 | 69.9192 |
| 0.6499 | 0.829686 | 0.04623 | 1206.36 | -41.6613 | 828.1940 | 69.4682 |
| 0.7005 | 0.826710 | 0.03913 | 1209.81 | -36.4998 | 826.4422 | 65.4753 |
| 0.7509 | 0.823663 | 0.03056 | 1214.17 | -30.3808 | 823.5528 | 56.9509 |
| 0.7998 | 0.820620 | 0.02137 | 1217.34 | -25.4502 | 822.3073 | 47.7023 |
| 0.8499 | 0.817383 | 0.01413 | 1221.22 | -19.7085 | 820.3262 | 35.6264 |
| 0.8999 | 0.814042 | 0.00732 | 1225.87 | -13.1391 | 817.4559 | 23.8460 |
| 0.9501 | 0.810541 | 0.00433 | 1230.19 | -6.8273 | 815.2309 | 12.4534 |
| 1.0000 | 0.806954 | 0.0000 | 1234.97 | 0.0000 | 812.5281 | 0.0000 |
| T/K = 303.15 |  |  |  |  |  |  |
| 0.0000 | 0.857594 | 0.0000 | 1246.70 | 0.0000 | 750.2299 | 0.0000 |
| 0.0476 | 0.855545 | 0.0119 | 1237.74 | -7.8946 | 762.9539 |  |
| 0.1000 | 0.853233 | 0.0249 | 1227.51 | -16.9214 | 777.8257 | 0.0000 |
| 0.1517 | 0.85901 | 0.0360 | 1216.99 | -26.2214 | 793.500 | 4.5971 |
| 0.2005 | 0.848632 | 0.0478 | 1208.19 | -33.8389 | 807.2538 | 12.2197 |
| 0.2499 | 0.846295 | 0.0568 | 1199.13 | -41.6699 | 821.7613 | 17.5788 |
| 0.3001 | 0.843871 | 0.0640 | 1192.03 | -47.4867 | 833.9683 | 26.0977 |
| 0.3501 | 0.841398 | 0.0699 | 1187.00 | -51.2029 | 843.5233 | 32.9978 |
| 0.4005 | 0.838855 | 0.0732 | 1184.06 | -52.7810 | 850.2873 | 39.2728 |
| 0.4509 | 0.836260 | 0.0737 | 1184.05 | -51.3896 | 852.9402 | 46.9593 |
| 0.5003 | 0.833661 | 0.0717 | 1185.48 | -48.5461 | 853.5364 | 52.6390 |
| 0.5500 | 0.830981 | 0.0684 | 1188.09 | -44.4723 | 852.5311 | 59.0887 |
| 0.6003 | 0.828188 | 0.0648 | 1191.34 | -39.6964 | 850.7454 | 64.5681 |
| 0.6499 | 0.825387 | 0.0567 | 1194.02 | -35.4659 | 849.8048 | 68.2924 |
| 0.7005 | 0.822431 | 0.0495 | 1198.07 | -29.7851 | 847.1028 | 69.9229 |
| 0.7509 | 0.819388 | 0.0430 | 1201.11 | -25.0692 | 845.9503 | 67.3218 |
| 0.7998 | 0.816371 | 0.0331 | 1204.59 | -19.9116 | 844.1778 | 61.7825 |
| 0.8499 | 0.813168 | 0.0245 | 1209.18 | -13.5477 | 841.0810 | 53.4974 |
| 0.8999 | 0.809861 | 0.0163 | 1211.48 | -9.4188 | 841.3119 | 42.7464 |
| 0.9501 | 0.806418 | 0.0094 | 1215.38 | -3.6209 | 839.4902 | 9.46787 |
| 1.0000 | 0.802900 | 0.0000 | 1217.05 | 0.0000 | 840.8561 | 0.0000 |
| T/K = 308.15 |  |  |  |  |  |  |
| 0.0000 | 0.851102 | 0.0000 | 1227.710 | 0.0000 | 777.6315 | 0.0000 |
| 0.0476 | 0.848792 | 0.0174 | 1221.640 | -5.4047 | 787.2849 | 3.7408 |
| 0.1000 | 0.846463 | 0.0333 | 1212.290 | -14.0034 | 801.6516 | 9.8924 |
| 0.1517 | 0.844186 | 0.0473 | 1204.000 | -21.5316 | 814.9652 | 14.9663 |
| 0.2005 | 0.841861 | 0.0633 | 1194.970 | -29.8231 | 829.5601 | 21.3236 |
| 0.2499 | 0.839445 | 0.0738 | 1187.170 | -36.8556 | 842.818 | 27.9754 |
| 0.3001 | 0.837012 | 0.0829 | 1181.840 | -41.3843 | 852.8848 | 34.3764 |
| 0.3501 | 0.834494 | 0.0866 | 1176.480 | -45.9238 | 863.1757 | 41.7811 |
| 0.4005 | 0.831945 | 0.0898 | 1173.880 | -47.6732 | 869.6197 | 49.7732 |
| 0.4509 | 0.829395 | 0.0874 | 1173.890 | -46.7879 | 872.2693 | 55.9658 |
| 0.5003 | 0.826748 | 0.0823 | 1174.800 | -44.9950 | 873.5962 | 62.4861 |
| 0.5500 | 0.824001 | 0.0779 | 1178.470 | -40.4108 | 870.9431 | 64.8935 |
| 0.6003 | 0.82121 | 0.0719 | 1181.900 | -36.0277 | 868.782 | 65.9461 |
| 0.6499 | 0.818274 | 0.0658 | 1186.570 | -30.3892 | 864.8864 | 63.0999 |
| 0.7005 | 0.815256 | 0.0597 | 1190.830 | -25.1105 | 861.7905 | 56.2796 |
| 0.7509 | 0.812257 | 0.0537 | 1194.400 | -20.4935 | 859.8178 | 49.6022 |
| 0.7998 | 0.809094 | 0.0450 | 1198.150 | -15.6956 | 857.5988 | 39.5907 |
| 0.8499 | 0.805831 | 0.0351 | 1201.660 | -11.0773 | 855.9291 | 28.1193 |
| 0.8999 | 0.802445 | 0.0254 | 1204.260 | -7.3347 | 855.6881 | 18.0281 |
| 0.9501 | 0.799013 | 0.0155 | 1207.600 | -2.8089 | 854.552 | 6.8396 |
| 1.0000 | 0.79800 | 0.0000 | 1209.190 | 0.0000 | 855.9671 | 0.0000 |
| T/K = 313.15 |  |  |  |  |  |  |
| 0.0000 | 848.752 | 0.0000 | 1209.340 | 0.0000 | 805.6054 | 0.0000 |
| 0.0476 | 846.636 | 0.0275 | 1203.430 | -4.9752 | 815.5707 | 3.1589 |
| 0.1000 | 844.326 | 0.0465 | 1195.960 | -11.3894 | 828.0499 | 7.5044 |
| 0.1517 | 841.962 | 0.0684 | 1188.700 | -17.5789 | 840.5489 | 13.0913 |
| 0.2005 | 839.733 | 0.0804 | 1181.370 | -23.8712 | 853.2708 | 19.5303 |
| 0.2499 | 837.428 | 0.0910 | 1172.810 | -31.3527 | 868.1549 | 24.5028 |
| 0.3001 | 835.047 | 0.0982 | 1164.470 | -38.5665 | 883.1459 | 30.8884 |
| 0.3501 | 832.643 | 0.1008 | 1159.080 | -42.8035 | 893.9523 | 38.3730 |
| 0.4005 | 830.164 | 0.1017 | 1156.180 | -44.5081 | 901.1253 | 46.7528 |
| 0.4509 | 827.628 | 0.1005 | 1155.800 | -43.658 | 904.4810 | 54.3425 |
| 0.5003 | 825.086 | 0.0973 | 1156.560 | -41.6572 | 906.0756 | 60.8918 |
| 0.5500 | 822.461 | 0.0930 | 1159.670 | -37.2622 | 904.0987 | 63.7123 |
| 0.6003 | 819.727 | 0.0884 | 1163.420 | -32.1726 | 901.2758 | 64.7337 |
| 0.6499 | 816.976 | 0.0803 | 1167.670 | -26.5613 | 897.7398 | 61.8142 |
| 0.7005 | 814.073 | 0.0732 | 1171.310 | -21.4894 | 895.3502 | 55.1109 |
| 0.7509 | 811.098 | 0.0650 | 1174.210 | -17.1179 | 894.2009 | 44.1269 |
| 0.7998 | 808.126 | 0.0562 | 1176.190 | -13.6647 | 894.4704 | 33.0806 |
| 0.8499 | 804.989 | 0.0464 | 1179.070 | -9.2268 | 893.5747 | 24.0512 |
| 0.8999 | 801.783 | 0.0332 | 1181.340 | -5.3506 | 893.7033 | 15.3614 |
| 0.9501 | 798.442 | 0.0214 | 1182.760 | -2.2636 | 895.2892 | 6.6393 |
| 1.0000 | 795.09 | 0.0000 | 1183.310 | 0.0000 | 898.2281 | 0.0000 |
| T/K = 318.15 |  |  |  |  |  |  |
| 0.0000 | 844.322 | 0.0000 | 1192.050 | 0.0000 | 833.4949 | 0.0000 |
| 0.0476 | 842.177 | 0.0346 | 1188.290 | -2.8355 | 840.9143 | 3.1499 |
| 0.1000 | 839.842 | 0.0602 | 1182.920 | -7.1612 | 850.9257 | 5.3145 |
| 0.1517 | 837.521 | 0.0788 | 1175.480 | -13.5425 | 864.1195 | 10.0478 |
| 0.2005 | 835.296 | 0.0930 | 1168.270 | -19.7261 | 877.1485 | 14.5571 |
| 0.2499 | 832.999 | 0.1052 | 1160.630 | -26.2993 | 891.1851 | 20.1052 |
| 0.3001 | 830.651 | 0.1106 | 1153.060 | -32.7555 | 905.4774 | 26.5904 |
| 0.3501 | 828.261 | 0.1140 | 1146.960 | -37.7149 | 917.775 | 34.2188 |
| 0.4005 | 825.799 | 0.1154 | 1144.110 | -39.3825 | 925.103 | 41.9123 |
| 0.4509 | 823.287 | 0.1139 | 1143.580 | -38.6957 | 928.786 | 50.2051 |
| 0.5003 | 820.752 | 0.1125 | 1144.300 | -36.7483 | 930.4826 | 56.0752 |
| 0.5500 | 818.154 | 0.1075 | 1146.820 | -32.9572 | 929.3396 | 58.9429 |
| 0.6003 | 815.457 | 0.1009 | 1150.800 | -27.6520 | 925.9749 | 59.7848 |
| 0.6499 | 812.722 | 0.0937 | 1154.410 | -22.6953 | 923.2893 | 56.8540 |
| 0.7005 | 809.859 | 0.0845 | 1157.930 | -17.7588 | 920.9286 | 48.7977 |
| 0.7509 | 806.909 | 0.0762 | 1160.720 | -13.5129 | 919.8574 | 38.6477 |
| 0.7998 | 803.971 | 0.0662 | 1162.920 | -9.8554 | 919.7291 | 28.5782 |
| 0.8499 | 800.864 | 0.0559 | 1164.400 | -6.8341 | 920.9517 | 19.366 |
| 0.8999 | 797.676 | 0.0437 | 1165.980 | -3.6649 | 922.1281 | 10.1095 |
| 0.9501 | 794.421 | 0.0249 | 1165.860 | -2.1356 | 926.097 | 3.9816 |
| 1.0000 | 791.126 | 0.0000 | 1166.300 | 0.0000 | 929.2526 | 0.0000 |
| T/K = 323.15 |  |  |  |  |  |  |
| 0.0000 | 0.839846 | 0.0000 | 1176.820 | 0.0000 | 859.7660 | 0.0000 |
| 0.0476 | 0.837632 | 0.0479 | 1174.800 | -1.0448 | 865.0055 | 0.6267 |
| 0.1000 | 0.835297 | 0.0765 | 1169.530 | -5.2131 | 875.2585 | 3.6499 |
| 0.1517 | 0.832968 | 0.0993 | 1163.450 | -10.1762 | 886.9032 | 6.2204 |
| 0.2005 | 0.830732 | 0.1178 | 1157.060 | -15.4834 | 899.1400 | 11.1562 |
| 0.2499 | 0.828484 | 0.1257 | 1149.720 | -21.6980 | 913.1281 | 15.6825 |
| 0.3001 | 0.826143 | 0.1329 | 1142.930 | -27.3129 | 926.6282 | 21.9617 |
| 0.3501 | 0.823778 | 0.13570 | 1137.450 | -31.5896 | 938.2643 | 30.2607 |
| 0.4005 | 0.821342 | 0.1363 | 1133.630 | -34.1621 | 947.3998 | 37.6227 |
| 0.4509 | 0.818.851 | 0.1347 | 1133.210 | -33.2983 | 950.9864 | 44.5644 |
| 0.5003 | 0.816363 | 0.1298 | 1133.420 | -31.7933 | 953.5313 | 50.4236 |
| 0.5500 | 0.813786 | 0.1250 | 1135.720 | -28.1520 | 952.6804 | 52.7146 |
| 0.6003 | 0.8110963 | 0.1204 | 1138.630 | -23.8438 | 950.9602 | 53.9218 |
| 0.6499 | 0.808403 | 0.1107 | 1141.760 | -19.2928 | 948.9043 | 49.4448 |
| 0.7005 | 0.805566 | 0.1012 | 1145.410 | -14.1481 | 946.1869 | 42.3020 |
| 0.7509 | 0.802647 | 0.0921 | 1147.820 | -10.2018 | 945.6444 | 33.1900 |
| 0.7998 | 0.799761 | 0.0786 | 1149.150 | -7.33381 | 946.8612 | 23.4044 |
| 0.8499 | 0.796692 | 0.0668 | 1150.670 | -4.18727 | 947.9992 | 15.2110 |
| 0.8999 | 0.793546 | 0.0527 | 1150.710 | -2.47017 | 951.6913 | 7.7372 |
| 0.9501 | 0.790328 | 0.0327 | 1176.820 | 0.0000 | 955.1679 | 1.5979 |
| 1.0000 | 0.787126 | 0.0000 | 1174.800 | -1.0448 | 961.2237 | 0.0000 |

Standard uncertainty, *u*: *u* (*T*) = 1·10−2 K, *u* (*ρ*) = 2.9·10–2 kg⋅m–3, *u* (*u*) = 1.3·10–1 m·s–1

The variations in the *V*mE values as a function of the mole fractions of 1-butanol or 1-pentanol at *T* = (298.15, 303.15, 308.15, 313.15, 318.15, and 323.15) K is shown in Figures 1 and 2, and has been calculated using the following relation:

(1)

Fig. 1. Excess Molar Volume (*V*mE) of EB(x1) + But -OH(x2) system for different molar ratios at different temperatures.

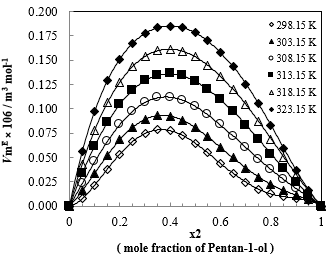


Fig. 2. Excess Molar Volume (*V*mE) of EB(x1) + PL(x2) system for different molar ratios at different temperatures.

In Eq. 1, the *x*1, *M*1, and *ρ*1 represent, respectively, mole fraction, molar mass, and experimental density of ethyl benzene, while the corresponding quantities of 1-alkanols are denoted by *x*2, *M*2, and *ρ*2. The *V*mE values at each of the studied temperatures have been fitted to a Redlich-Kister-type smoothing equation of the following form [21]:

(2)

The *Y* refers to *V*mE, and the mole fractions of ethylbenzene and 1-alkanols are expressed by *x*1 and *x*2 in Eq. 2. The variable *Ai* represents the equation coefficients (Table 4), which have been obtained by fitting the equation to the experimental values with a least-square regression method and are summarized with standard deviation at each studied temperature.

Table 4. Coefficients, *Ai*, of Redlich–Kister equation (Eq 10), expressing excess molar volumes, *V*mE*,* deviation in ultrasonic speeds, Δ*u*, deviation in isentropic compressibility, Δ*κs*, and standard deviation *σ*  for the binary mixtures of ethylbenzene (1) with butan-1-ol (2) or pentan-1-ol (2) at *T* = (298.15 to 323.15) K.

| *T*/K | | *A0* | | *A1* | | *A2* | | *A3* | *σ* | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ethylbenzene (1) + Butan-1-ol (2) | | | | | | | | | | |
| *V*mΕ·106/m3 ∙ mol−1 *σ* (m3∙mol−1) | | | | | | | | | | |
| 298.15 | | 0.248 | | –0.135 | | –0.131 | | 0.079 | 0.0012 | |
| 303.15 | | 0.288 | | –0.096 | | –0.095 | | 0.065 | 0.0007 | |
| 308.15 | | 0.336 | | –0.166 | | –0.002 | | 0189 | 0.0013 | |
| 313.15 | | 0.390 | | –0.159 | | –0.111 | | 0.091 | 0.0012 | |
| 318.15 | | 0.442 | | –0.159 | | –0.180 | | 0.058 | 0.0017 | |
| 323.15 | | 0.517 | | –0.186 | | –0.292 | | 0.005 | 0.0026 | |
| *μ*m.s-1  *σ* (m∙ s−1) | | | | | | | | | | |
| 298.15 | | –213.24 | 104.57 | | | 32.47 | | –84.06 | 0.723 | |
| 303.15 | | –195.88 | 120.97 | | | 78.54 | | –108.49 | 0.727 | |
| 308.15 | | –177.56 | 118.13 | | | 101.02 | | –117.29 | 0.519 | |
| 313.15 | | –163.93 | 117.26 | | | 122.75 | | –135.48 | 1.091 | |
| 318.15 | | –144.79 | 138.29 | | | 112.04 | | –147.80 | 0.861 | |
| 323.15 | | –124.85 | 143.35 | | | 97.06 | | –128.99 | 0.764 | |
| *κ*sE/TPa−1 *σ* (TPa−1) | | | | | | | | | | |
| 298.15 | | 270.68 | | –62.54 | | –126.63 | | 119.17 | 0.948×10-12 | |
| 303.15 | | 260.22 | | –156.57 | | –125.13 | | 155.64 | 1.054×10-12 | |
| 308.15 | | 245.88 | | –161.59 | | –156.58 | | 172.34 | 0.839×10-12 | |
| *T*/K | *A0* | | | | *A1* | | *A2* | *A3* | | *σ* | |
| 313.15 | 238.73 | | | | –168.21 | | –194.93 | 205.22 | | 1.769×10-12 | |
| 318.15 | 219.94 | | | | –167.64 | | –223.19 | 228.19 | | 1.527×10-12 | |
| 323.15 | 197.06 | | | | –150.58 | | –236.75 | 202.85 | | 1.414×10-12 | |
| Ethyl benzene (1) + Pentan-1-ol (2) | | | | | | | | | | | |
| *V*mΕ·106/m3 ∙ mol−1 *σ* (m3∙mol−1) | | | | | | | | | | | |
| 298.15 | 0.259 | | | | –0.366 | | –0.149 | 0.427 | | 0.0012 | |
| 303.15 | 0.323 | | | | –0.345 | | –0.117 | –0.295 | | 0.0015 | |
| 308.15 | 0.411 | | | | –0.305 | | –0.093 | 0.179 | | 0.0023 | |
| 313.15 | 0.513 | | | | –0.276 | | –0.057 | 0.027 | | 0.00261 | |
| 318.15 | 0.614 | | | | –0.288 | | –0.004 | –0.046 | | 0.00259 | |
| 323.15 | 0.713 | | | | –0.273 | | 0.047 | –0.232 | | 0.0028 | |
| *μ*m.s-1 *σ* (m∙ s−1) | | | | | | | | | | | |
| 298.15 | –71.30 | | | | 5.24 | | –24.84 | –5.05 | | 0.271 | |
| 303.15 | –67.24 | | | | 4.29 | | 10.059 | 5.342 | | 0.265 | |
| 308.15 | –59.06 | | | | 6.93 | | 32.798 | –3.03 | | 0.248 | |
| 313.15 | –51.18 | | | | 11.76 | | 40.94 | –15.12 | | 0.129 | |
| 318.15 | –44.22 | | | | 11.49 | | 47.11 | –15.09 | | 0.109 | |
| 323.15 | –37.50 | | | | 15.18 | | 50.80 | –22.81 | | 0.190 | |
| *κ*sE/TPa−1 *σ* (TPa−1) | | | | | | | | | | | |
| 298.15 | 84.74 | | | | –5.61 | | 27.45 | 9.85 | | 0.325×10-12 | |
| 303.15 | 84.42 | | | | –4.84 | | –15.53 | –5.48 | | 0.326×10-12 | |
| 308.15 | 78.33 | | | | –8.78 | | –45.94 | 3.67 | | 0.313×10-12 | |
| 313.15 | 71.93 | | | | –16.22 | | –58.92 | 19.62 | | 0.178×10-12 | |
| 318.15 | 65.89 | | | | –16.93 | | –70.13 | 19.73 | | 0.172×10-12 | |
| 323.15 | 58.47 | | | | –23.18 | | –78.13 | 30.48 | | 0.316×10-12 | |

The standard deviation values have been calculated using the following equation, which comprises *n* as the number of experimental points, *p* as the number of coefficients of Eq. 2, and *Y*expt and *Y*calc as the experimental and calculated values of the properties.

(3)

Generally, the values of the excess functions *V*mE depend upon several physical and chemical contributions [3,17]. The physical contribution depends mainly on two factors, namely,

(a) The dispersion forces or weak dipole-dipole interaction that leads to positive values,

(b) The geometrical effect allows the fitting of molecules of two different sizes into each other's structure, resulting in negative values.

The chemical contributions include the breaking up of the associates present in pure liquids, resulting in positive *V*mE. In the present mixture *V*mE value for (EB + 1-butanol or 1-pentanol) binary mixtures is positive over the whole composition range (Figures 1 and 2). When a small amount of 1-alkanols is added to ethyl benzene separately, it is expected that it would disperse within aromatic hydrocarbons, causing depolymerization of the network structures and disrupting their H-bonding and resulting in volume expansion. The experimental data and the derived quantities have been used to understand the intermolecular interactions, particularly the interaction (π….H) between π–electrons of ethyl benzene and H-atom of –OH group of 1-alkanols and the interaction (π – π) between the π–electrons of ethyl benzene and 1-alkanols. Therefore, the analysis of *η* and *σ* in (1-alkanols+ ethyl benzene) mixtures is a valuable source of information that may be used to examine the relation between the internal structure of the system and its physical properties. Here, the observed *VmE* becomes positive for all binary mixtures. Similar conclusions were discussed for the binary mixtures of 1-propanol + aromatic hydrocarbons [24]**,** mesitylene + alkanol [25], 1-nonanol + ethyl benzene [26], butanol isomers + hydrocarbons [27]. It has also been found that the *VmE* values for ethyl benzene with 1-alkanols become more positive with the rise of temperature, *i.e.,* *δVmE/δT* are positive. The order of excess molar volume values was pentan-1-ol > butan-1-ol, suggesting higher positive deviation for longer chain alkan-1-ols. The self-associated alkan-1-ol molecules, as they remained in the pure state through hydrogen bonding, were disrupted when mixed with ethyl benzene via the π-electron donor-acceptor interactions between the aromatic ring and hydroxyl group [20].

The behavior of the excess functions may be suggested as follows: in this work, the common component, ethyl benzene, has a dipole moment of 0.58D. The other components of the binary mixtures are 1-alkanol. All these alkanols are protic molecules, and 1-pentanol has a larger dipole moment than 1- 1-butanol. It is observed that the interactions of EB in the systems follow the order of 1-pentanol**>**1-butanol.

**3.2. *Acoustic properties***

The ultrasonic speeds, *u*, deviation in ultrasonic speeds, Δ*u*, isentropic compressibility, *κs*, for the binary systems of EB with 1-butanol and 1-pentanol at different temperatures (298.15 to 323.15 K) with the interval of 5 K are compiled in Table 3.

The deviation in ultrasonic speeds, Δ*u*, isentropic compressibility, *κs*, have been computed using the following relations[18]:

Δ*u* = *uexp* ̶ (*φ1u1*+ *φ2u2*) (4)

*κs*= (*ρu*2)  ̶ 1 (5)

Δ*κs*= *κs*  ̶ (*φ1κs*1 + *φ2κs*2) (6)

In Eq. 4, the volume fraction and the ultrasonic speeds of EB are denoted as *φ*1 and *u*1, respectively, and *φ*2 and *u2* are the corresponding quantities of 1-alkanols. The density of the binary mixtures and the corresponding speeds of sound are expressed, respectively, with *ρ* and *u* in Eq. 5. At all temperatures, *u*of the pure liquids varies in the order Pen-OH > EB > Bu-OH.

The volume fraction was calculated from the individual pure molar volumes, *Vi*, and the corresponding mole fractions, *x*i, using the following relation:

(7)

The variation of Δ*u* vs mole fraction is shown in Figs. 3 and 4. Negative deviations in Δ*u* over the entire composition range for both the systems at all the temperatures studied suggest the presence of weak interaction dispersive forces between the unlike molecules. This may be due to the significant interactions of the type π….H between π-electrons of EB and H-atom of the –OH group of 1-butanol or 1-pentanol. Similar reports are made by Bahadur *et al.* [28] and Sumathi and Govindarajan [29]. According to their reports, the negative values of Δ*u* indicate a decrease in the strength of interaction between the molecules in the mixture. The composition dependence of Δ*u* is represented by the Redlich-Kister relation as shown in Eq. 2. The *Y* in Eq. 2 refers to Δ*u*, and the corresponding equation coefficients, *Ai*, are listed (Table 4).

Fig. 3. Deviation in sound velocity (Δ*u*) of EB(x1) + But-OH(x2) system for different molar ratios at different temperatures.

Fig. 4. Deviation in sound velocity (Δu) of EB(x1) + PL(x2) system for different molar ratios at different temperatures.

At all temperatures, *κs* of the pure liquid varies in the order Bu-OH > Pen-OH > EB. The variation of Δ*κs* vs mole fraction is shown in Figs. 5 and 6. The observed positive values of Δ*κs*for all the investigated systems over the entire composition range indicate the presence of weak interaction between the component molecules of the mixtures. Fort and Moore [30] suggested that positive deviations in Δ*κs*indicate the presence of weak interactions between the component molecules in the mixtures [16,31].

Fig. 5. Deviation in isentropic compressibility (Δ*κ*s) of EB(x1) + But-OH(x2) system for different molar ratios at different temperatures.

Fig. 6. Deviation in isentropic compressibility (Δκs) of EB(x1) + PL(x2) system for different molar ratios at different temperatures.

**4. Conclusion**

The present paper is a continuing effort towards the understanding of the mixing behavior of binary liquid mixtures comprising n-alkanols + ethyl benzene. The densities 𝜌, excess molar volumes *V*m𝐸, speeds of sound *𝑢*, and data of binary mixtures ethyl benzene with 1-butanol/1-pentanol have been reported at (298.15, 303.15, 308.15, 313.15, 318.15 and 323.15) K. The excess molar volumes *V*m𝐸 and deviation in isentropic compressibility Δ*κ𝑠*were evaluated using the experimental data of *ρ*, *η*, and *u* and correlated using the Redlich–Kister type polynomial equation. The derived acoustical parameters and their excess parameters Δ*κ𝑠* and *V*𝑚𝐸 are positive, and Δ*u* are negative, which hints at the presence of weak dispersive forces between the component molecules in the mixture at all six temperatures studied.

**Acknowledgments**

A. F. M. Sanaullah and M. A. Uddin acknowledge 'The Research and Publication cell, University of Chittagong' (196/2020) for allocating the financial grant to carry out this research. The authors also express their sincere thanks to the Department of Chemistry, University of Chittagong, Chittagong, for providing other necessary facilities to finish the present work.

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